AD 257 880

GCA TECHNICAL REPORT
60-5-N

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PHOTOIONIZATION OF ATOMIC OXYGEN AND NITROGEN

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CONTRACT NO. NASw-124

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
GODDARD SPACE FLIGHT CENTER
WASHINGTON, D.C.

DECEMBER 1960

N-61-3-4
XEROX

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A knowledge of the photoionization cross sections of atomic oxygen and atomic nitrogen from the spectral heads down to the x-ray region is necessary for the interpretation of the behavior of the ionized layers. ~~In this note we examine the~~ available theoretical and experimental data were examined and ~~obtain~~ sets of recommended values were obtained.

(1) <u>Atomic Oxygen</u>. The spectral head for atomic oxygen is at 911 A corresponding to the transition $O(4_S) + e$. There are discontinuities at 732 A and at 665 A corresponding to the transitions $O(3p)\ O^+ (2_D) + e$ and $O^+ (2p) + e$ respectively. The cross sections have been computed by Bates and Seaton[1] using the Hartree-Fock method for the initial and final states for wave lengths down to 460 A and we have used some less refined calculations of Dalgarno and Parkinson[2] to extrapolate the calculations of Bates and Seaton to shorter wave lengths.

There are also discontinuities associated with transitions in which the first state of O^+ is less an excited configuration, but these are unlikely to be significant, especially since they lie in a region in which transitions from the inner 2s shell are energetically possible (the first such transition occurs at 339 A).

According to Nicolet[3], the ionization limit for the ejection of a 2s electron lies at 125 A; but according to Dalgarno and

Parkinson[2], there are two ionization limits, one lying at 435 A and the other at 310 A. As Dalgarno and Parkinson remark, this is an important modification since the II resonance line is located at 304 A.

There are no very accurate values available of the cross sections at these limits but Dalgarno and Parkinson[2] have given some preliminary estimates of $1.3 \times 10^{-17} cm^2$ and $1.0 \times 10^{-17} cm^2$ at 435 A and 310 A respectively. Dalgarno and Parkinson have also given values at shorter wave lengths and in particular, at 68.0 A and 44.5 A for which they estimate cross sections of $4 \times 10^{-19} cm^2$ and $1.5 \times 10^{-19} cm^2$ (these estimates include the contribution from ionization of the 2p shell). Measurements have been made for molecular oxygen[4] at 68.0 A and at 44.5 A and if it is assumed that a molecule of oxygen is equivalent at these wave lengths to two atoms of oxygen, the measured cross sections are $4.32 \times 10^{-19} cm^2$ and $1.50 \times 10^{-19} cm^2$ in harmony with the theoretical estimates. We assume, therefore, that the values given by Dalgarno and Parkinson are accurate at all wave lengths. A more refined calculation is desirable, however.

According to Nicolet[3], the ionization limit for the ejection of a 1s electron lies at 21.5 A. Dalgarno and Parkinson adopt a limit of 22.8 A but the discrepancy is not significant (there are actually two limits which we do not distinguish). Dalgarno and Parkinson have made some approximate calculations at wave lengths shorter than 22.8 A but the agreement with the available experimental data (which refers again to O_2) is not very close and it seems better

to adopt the cross sections derived by Victoreen[5] which are of a semi-empirical kind designed to be in harmony with the measurements. This assumes that $O_2 \cong 20$ which must be closely satisfied for the tightly-bound 1s electrons. Despite the harmony between the experimental data and Victoreen's computations, the precise behavior of the cross section near the ionization limit is open to question. There are no observations between 22.8 A and 17.7 A and the cross section may pass through a maximum in this region. The cross section near the ionization limit is rather sensitive to the detailed nature of the final continuum wave function describing the ejected electron and a more refined theoretical analysis is required.

The recommended cross sections are collected together in the form of a table of values rather than as a figure since numerical values are required for ionospheric applications. Cross sections for O_2 for $\lambda < 300$ A may be obtained by multiplication by two. For longer wave lengths, measurements of total absorption by O_2 have been carried out by Weissler and Lee[6,7] and of photoionization of O_2 by Wainfran, Walker and Weissler[8] (see also Weissler, Samson, Ogawa, and Cook[9]).

(2) <u>Atomic Nitrogen</u>. The spectral head for atomic nitrogen lies at 852 A and cross sections have been computed by Bates and Seaton[1] using the Hartner-Fock method for the initial and final states for wave lengths down to 440 A. We have extrapolated them to shorter wave lengths as for atomic oxygen.

Table 1

PHOTOIONIZATION CROSS SECTIONS Q OF ATOMIC OXYGEN IN CM^2

Wavelength (A^o)	Q (cm^2)	Wavelength (A^o)	Q (cm^2)
911	2.6×10^{-18}	153	2.2×10^{-18}
769	3.4×10^{-18}	131	1.5×10^{-18}
732	3.5×10^{-18}	115	1.1×10^{-18}
		100	8.5×10^{-19}
		83	5.3×10^{-19}
		70	31.7×10^{-19}
		52	2.3×10^{-19}
732	7.6×10^{-18}	40	1.2×10^{-19}
665	8.6×10^{-18}	34	9.1×10^{-20}
		30	6.8×10^{-20}
		26	4.1×10^{-20}
		22.8	2.0×10^{-20}
665	1.1×10^{-17}		
587	1.3×10^{-17}		
525	1.3×10^{-17}		
475	1.3×10^{-17}	22.8	5.3×10^{-19}
455	1.1×10^{-17}	20	4.0×10^{-19}
435	9.8×10^{-18}	15	2.0×10^{-19}
		8	3.6×10^{-20}
		6	1.6×10^{-20}
		5	9.5×10^{-21}
		4	5.0×10^{-21}
435	1.3×10^{-17}	3	2.1×10^{-21}
400	1.2×10^{-17}	2.5	1.3×10^{-21}
365	1.0×10^{-17}	2.0	6.7×10^{-22}
315	8.0×10^{-18}	1.5	6.7×10^{-22}
310	7.8×10^{-18}	1.0	8.8×10^{-23}
		0.8	4.7×10^{-23}
		0.6	2.3×10^{-23}
		0.5	1.5×10^{-23}
		0.4	1.0×10^{-23}
310	1.0×10^{-17}	0.3	7.0×10^{-24}
290	9.2×10^{-18}	0.25	5.8×10^{-24}
270	8.0×10^{-18}	0.20	5.0×10^{-24}
245	6.3×10^{-18}	0.15	4.4×10^{-24}
220	5.1×10^{-18}	0.12	4.1×10^{-24}
185	3.4×10^{-18}	0.10	3.8×10^{-24}

We have not taken into account the discontinuities associated with final excited states of N^+. The first occurs at 376 A so that they all lie in the region in which ionization of the 2s shell is energetically possible.

According to Nicolet[3], the ionization limit for the ejection of a 2s electron lies at 175 A; but according to Dalgarno and Parkinson[2], there are two limits, one at 608 A and the other at 367 A. Thus, the helium line at 584 A can cause ionization from the 2s shell.

No very accurate values are available of the cross sections for the 2s shell ionization but Dalgarno and Parkinson have given some preliminary estimates. At 68.0 A and 44.5 A, they obtain $1 \times 10^{-19} cm^2$ and $6 \times 10^{-20} cm^2$. Assuming that $N_2 \cong 2N$, the measurements yield $2.5 \times 10^{-19} cm^2$ and $8.8 \times 10^{-20} cm^2$, values which are much larger than the theoretical estimates.

This is not necessarily any discrepancy and we incline to the view that the assumption that a nitrogen molecule is equivalent to two nitrogen atoms is invalid, the fact that a similar assumption apparently holds for oxygen being due to chance. However, it must be admitted that the theoretical estimates are not firmly based and an error by a factor of three is certainly possible. Again, a more refined theoretical examination is necessary. In the table, we give values computed by Dalgarno and Parkinson.

For the 1s shell ionization which commences at about 30.3 A, we merely reproduce the semi-empirical values given by Victoreen[5] with the remark that the values between 30.3 A and 17.7 A are open to question and further work in this region is required.

The recommended values are collected together in Table 2. We stress that they refer to atomic nitrogen. For wave lengths shorter than 30.3 A, cross sections for N_2 may be derived by multiplying by two but this is not a good approximation at longer wave lengths. Values for N_2 at longer wave lengths may be derived by interpolation amongst the values measured[4] at 44.5 Å and at 68 A and between 300 A and 1300 A (Weissler, Lee and Mohr[7]). The measurements do not refer only to photoionization cross sections, but to the total absorption cross sections.

Over a more limited range, photoionization cross sections of N_2 have been measured by Wainfan, Walker and Weissler[8] (see also Weissler, Samson, Ogawa, and Cook[9]).

Table 2

PHOTOIONIZATION CROSS SECTIONS Q OF ATOMIC NITROGEN IN CM^2

Wavelength (A°)	Q (cm^2)	Wavelength (A°)	Q (cm^2)
852	9.0×10^{-18}	63	9.9×10^{-20}
727	1.0×10^{-17}	49	7.0×10^{-20}
634	1.1×10^{-17}	34	4.1×10^{-20}
608	1.0×10^{-17}	30.3	3.2×10^{-20}
608	1.4×10^{-17}	30.3	7.0×10^{-19}
536	1.0×10^{-17}	20	2.6×10^{-19}
480	6.7×10^{-18}	15	1.2×10^{-19}
396	3.6×10^{-18}	10	4.0×10^{-20}
367	2.6×10^{-18}	6	9.3×10^{-21}
		5	5.5×10^{-21}
		4	2.9×10^{-21}
		3	1.2×10^{-21}
367	5.7×10^{-18}	2.5	7.2×10^{-22}
340	4.3×10^{-18}	2.0	3.7×10^{-22}
316	3.5×10^{-18}	1.5	1.6×10^{-22}
278	2.2×10^{-18}	1.0	5.1×10^{-23}
248	1.5×10^{-18}	0.8	2.8×10^{-23}
223	1.0×10^{-18}	0.6	1.5×10^{-23}
203	7.4×10^{-19}	0.5	1.0×10^{-23}
166	3.7×10^{-19}	0.4	7.2×10^{-24}
141	2.4×10^{-19}	0.3	5.3×10^{-24}
122	1.7×10^{-19}	0.25	4.7×10^{-24}
108	1.5×10^{-19}	0.20	4.2×10^{-24}
96	1.3×10^{-19}	0.15	3.8×10^{-24}
79	1.1×10^{-19}	0.12	3.5×10^{-24}
73	1.1×10^{-19}	0.10	3.3×10^{-24}

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